

Summer 2016 NSERC USRA Report The Hard Square Constraint

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Consider the set of binary strings of length n with no adjacent “1” s, denoted at c_n . The quantity which we are most interested in computing is known as the **growth rate** of c_n , defined as $\lim_{n \rightarrow \infty} \|c_n\|^{\frac{1}{n}}$. Such strings may be constructed by recording the label vertexes reached in a path of length $n - 1$ on the graph G in Figure 1.

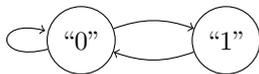


Figure 1: A graph G whose paths construct sequences in c_n

It is known that the growth rate of c_n is the largest eigenvalue of the adjacency matrix of G , namely $\frac{1+\sqrt{5}}{2}$. Hence, the set X is known as the **golden mean shift**. The logarithm of the growth rate is known as the (topological) **entropy** of the shift. Quantities such as entropy and the growth rate are used in information and coding theory. In general, the growth rate of a large class of 1-dimensional constraints, including the golden mean shift, which can be expressed as a graph can be computed in closed form. Much of the theory behind these **sofic shifts** is detailed in [1].

However, computation of growth rates in higher dimensions remains unsolved. The two-dimensional analogue of the golden mean shift forbids adjacent 1s horizontally or vertically in a binary two-dimensional $m \times n$ array. This is known as the **hard square constraint**. The analogue of the growth rate, also known as the **hard square constant** η is defined as

$$\eta = \lim_{m,n \rightarrow \infty} f_{m,n}^{\frac{1}{mn}} \tag{1}$$

where $f_{m,n}$ is the number of $m \times n$ arrays obeying the hard square constraint. However, there are a number of techniques based on linear algebra, detailed in [2], [3], and [4], which have obtained rigorous bounds of η . The most accurate result is that $\eta = 1.503048082475332264\dots$. Re-implementation of these methods formed the initial part of the authors' summer research.

Now suppose we would like to give a weight to each hard square configurations. A configuration τ is weighted by $z^{1(\tau)}$ where $1(\tau)$ is the number of 1s in τ and z is a real-valued parameter. Such a weight denotes the energy of the configuration τ . Then, the total weight of configurations is known as the **partition function**, defined as:

$$Z_{mn}(z) = \sum_{\tau \in \mathcal{R}_{m,n}} z^{1(\tau)} \tag{2}$$

where $\mathcal{R}_{m,n}$ denotes the set of all $m \times n$ hard square configurations. The weight z controls the configurations whose terms dominate the sum in $Z_{mn}(z)$. For low z , the configurations τ which dominate the partition function mirror a gas, whereas for large z , these configurations mirror a crystal. It is estimated in [5] that there is a phase transition z_c between these two states at around 3.7962 ± 0.0001 .

The **free energy** $\kappa(z)$ is then the analogue of the hard square constant when hard square configurations are weighted, defined as

$$\kappa(z) = \lim_{m,n \rightarrow \infty} Z_{mn}(z)^{\frac{1}{mn}} = \lim_{n \rightarrow \infty} Z_{nn}(z)^{\frac{1}{n^2}} \quad (3)$$

We conjecture that the free energy $\kappa(z)$ is related to a number of probabilities related to broken boxes. Using computational tools to come to these conjectures was the main work of the summer. A **broken box** with dimensions $a \times b \times c$ consists of a $a \times b$ next to a $(a+1) \times c$ rectangle. We may impose the hard square constraint on broken boxes, and along with differing boundary conditions on the boxes. Free boundary conditions are illustrated on the left and checkboard boundary conditions are illustrated on the right in the following figure:

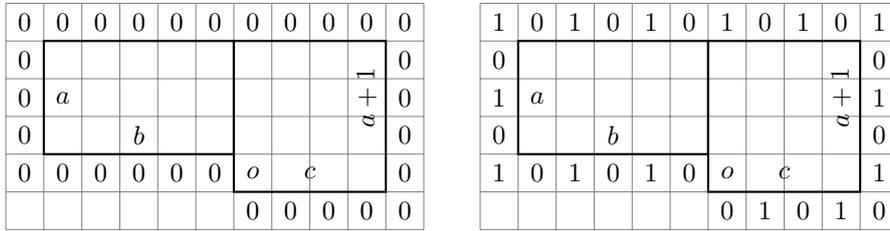


Figure 2: Broken boxes with free boundary condition (left) and checkboard boundary condition (right) with origin marked at o

Given free boundary conditions, we found that the limiting probability $P_{f,\mathcal{B}}(z)$ that the origin is zero as the dimensions a, b, c get large does not exist for large z . Such probabilities are defined by the partition function $Z_{a,b,c}(z)$ over all possible configurations on a broken box. However, two subsequences over lattices with odd and even number of sites respectively have limits $P_{f,\mathcal{B}}^e(z)$ and $P_{f,\mathcal{B}}^o(z)$. We propose that

Conjecture 1. For all $z > 0$, $\kappa(z) = \frac{1}{\sqrt{P_{f,\mathcal{B}}^e(z)P_{f,\mathcal{B}}^o(z)}}$.

This extends a known theorem that $\kappa(z) = \frac{1}{P_{f,\mathcal{B}}(z)}$ for sufficiently small z , as the odd and even subsequences yield the same limit when z is small.

Given checkboard boundary conditions, we found that the limiting probability $P_{c,\mathcal{B}}(z)$ that the origin is one as dimensions a, b, c get large is related to $\kappa(z)$ as follows:

Conjecture 2. For all $z > 0$, $\kappa(z) = \sqrt{\frac{z}{P_{c,\mathcal{B}}(z)}}$

Conjecture 2 is known for $z < 2.48$ and $z > 468$ by [6], but our computations seem to suggest that it holds for all $z > 0$. Evidence from series expansions of $\kappa(z)$ supports the conjecture in addition to computed approximations of $P_{c,\mathcal{B}}(z)$.

Finally, we propose that Conjectures 1 and 2 continue to hold when we consider the limiting probability the origin of a rhombus is 0 (resp. 1) instead of a broken box. A rhombus is a ball from the origin under the taxicab, or graph metric.

Overall, we have enjoyed our time working as USRA students with the mathematics department. We are grateful to Dr. Marcus and Dr. Briceño for aiding with the theoretical aspects of this work and Dr. Rechnitzer for help with the computational aspects of this work. We were particularly pleased by the freedom we had to explore different aspects of combinatorics and statistical mechanics through computational and theoretical lens, and will surely continue our investigations in the future. A more detailed account of our work this summer is available on request to adrian.she@alumni.ubc.ca or arman.raina@gmail.com.

References

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